

Modeling Impurity Concentration in Liquid Argon Detectors

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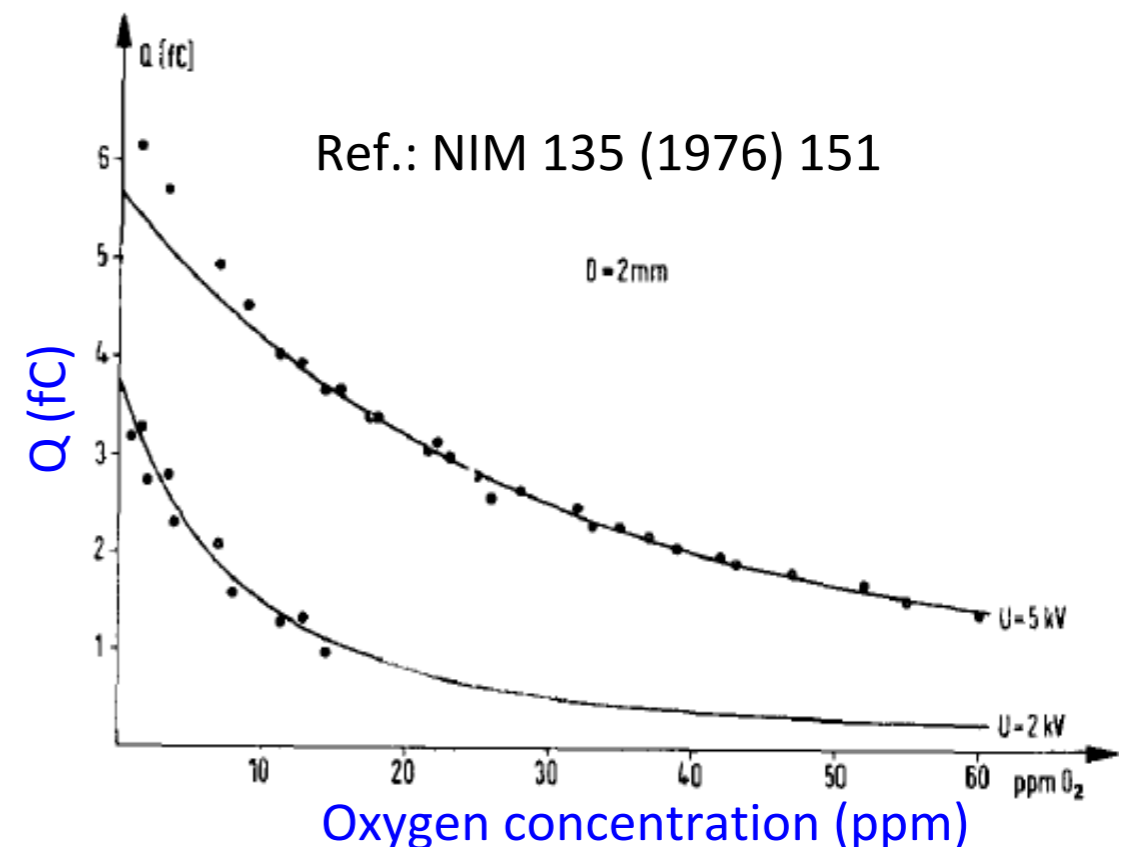
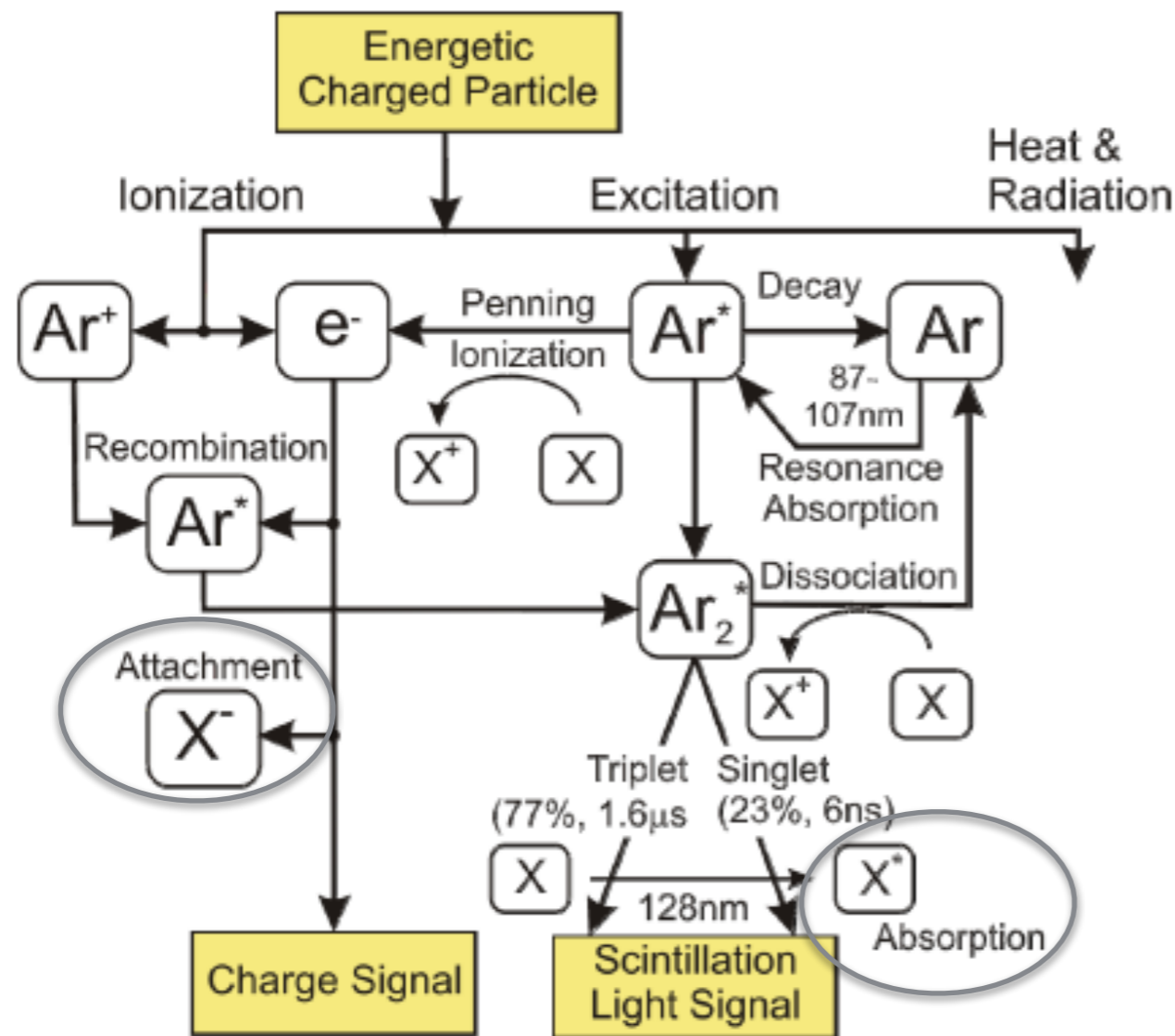


Outline

- Motivation
- Model description
- Measurement of Henry's coefficients for oxygen
- Determination of impurity leak rate
- Summary

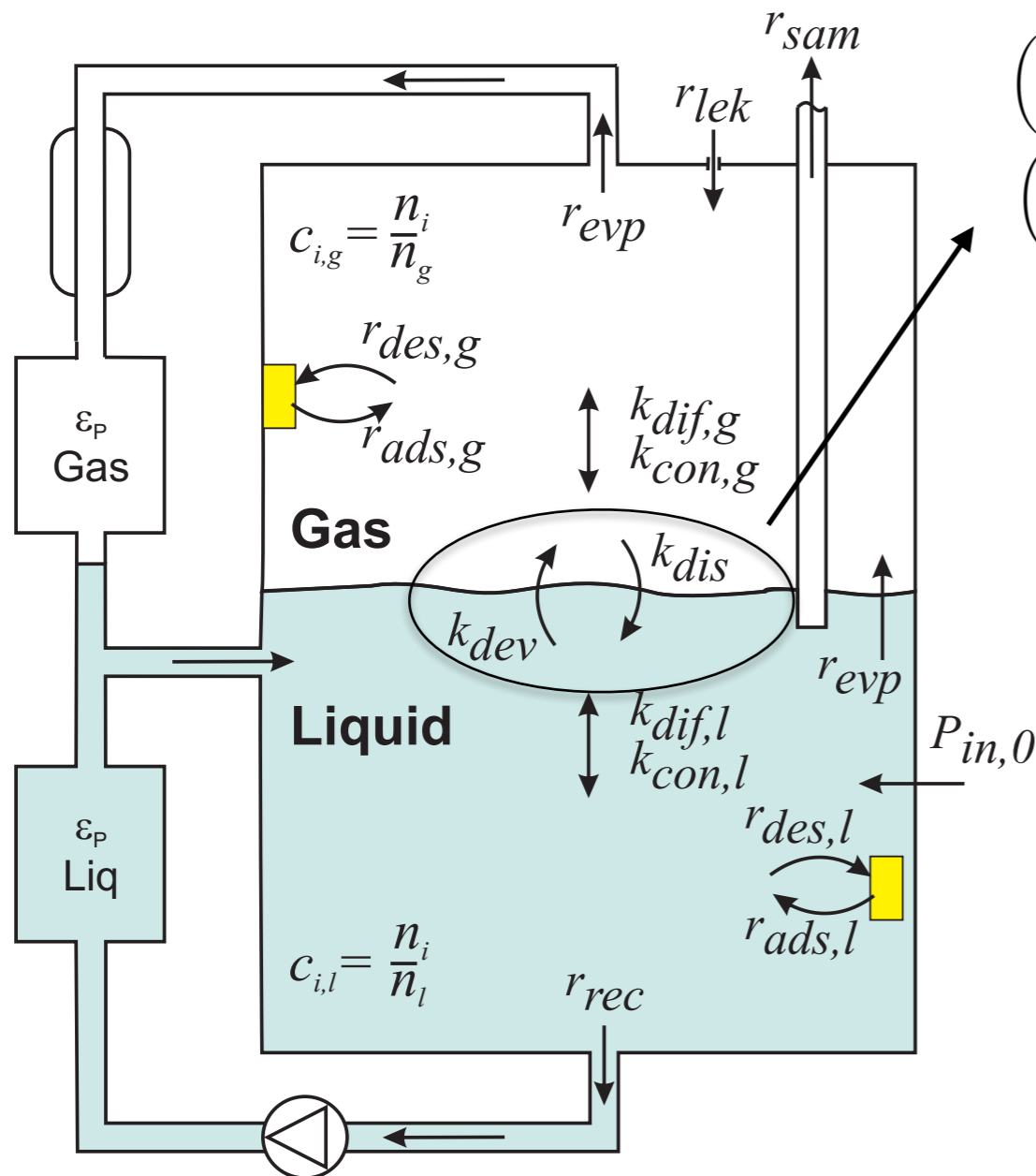
Motivation

- Impurities in LAr (O₂, H₂O, etc.) significantly reduce charge and light signals
- Ultra-high purity LAr (<1 ppb) required for long drift distances (> 3.6 m)
- A model is helpful to understanding the dynamics of impurities in LAr
- Useful for detector optimization and operation



Model Description

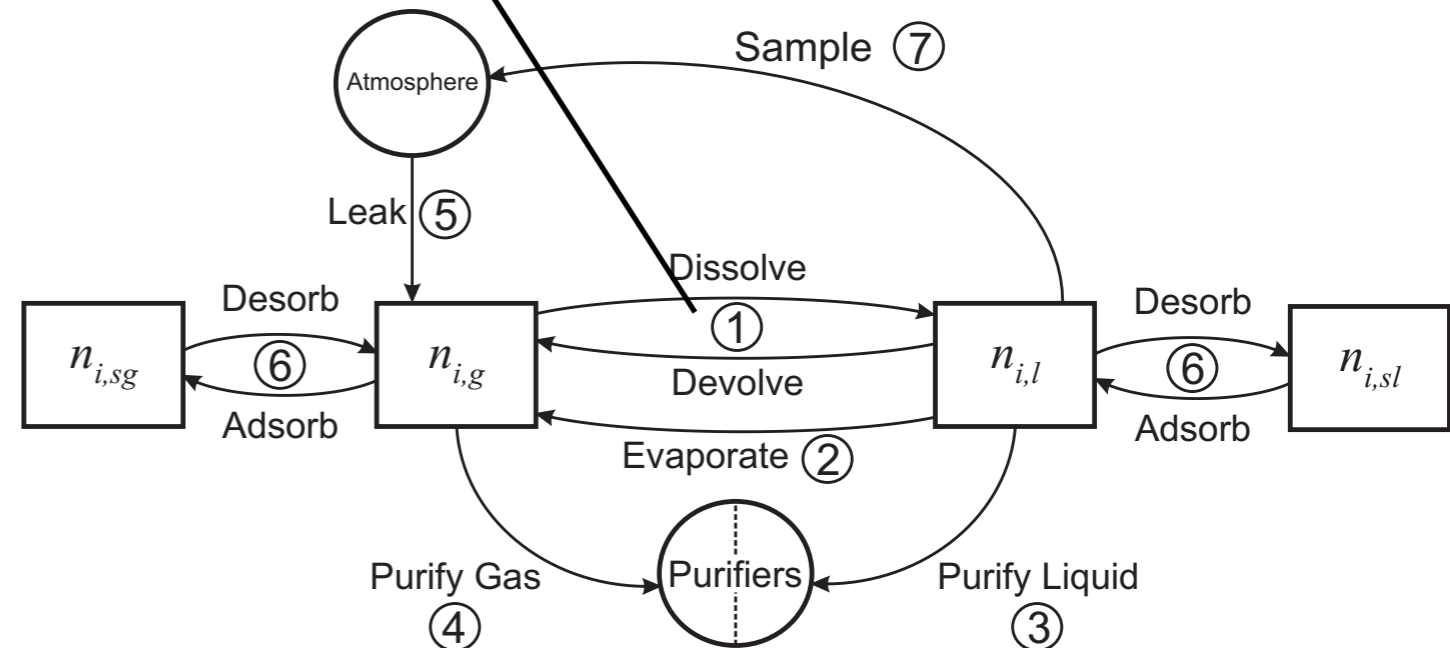
- Ultra-high purity (< 1.0 ppb for O₂, H₂O) is essential to operate LArTPC with long drift distances
- A quantitative kinetic model of impurity distribution is constructed
- Each process can be described by the an ordinary differential equation
- The entire system is the sum of all 7 processes



$$\left(\frac{dn_{i,g}}{dt}\right)_1 = n_g(-c_{i,g} \cdot k_{dis} + c_{i,l} \cdot k_{dev}),$$

$$\left(\frac{dn_{i,l}}{dt}\right)_1 = -\left(\frac{dn_{i,g}}{dt}\right)_1,$$

n_p , quantity of GAr (LAr)
 $n_{i,p}$, quantity of impurity in GAr (LAr)
 $c_{i,p} = n_{i,p}/n_p$, concentration of impurity in GAr (LAr)
 k_{dis}, k_{dev} , rate constant for dissolving/devolving impurity



Model Prediction

- Concentrations are in non-linear 3rd ODE
- Full formula derivations can be found in the full paper: [arXiv:2009.10906](https://arxiv.org/abs/2009.10906)
- Analytic solutions from outgassing (#6) and sampling (#7):

$$c_{i,l}(t) = c_{i,l}^{ss} + C_1 \cdot e^{-k_F t} + C_2 \cdot e^{-k_S t},$$

$$c_{i,g}(t) = c_{i,g}^{ss} + C_3 \cdot e^{-k_F t} + C_4 \cdot e^{-k_S t}.$$

Ultimate concentration Fast Components (~secs) Slow concentration (~hrs)

- Henry's constant is the partition of an impurity between liquid and gas phases

- The model predicts a way to measure Henry's Coefficient
- $$H_{xx}(T) = \frac{\text{Cleaning Rate of Ar}}{\text{Evaporation rate of LAr}}$$

$$H_{xx}(T) = \frac{c_{i,g(as)}}{c_{i,l(liquid)}}$$

Henry's coefficient at equilibrium

$$H_{xx}(T) = \frac{k_s \cdot n_{i,l}}{r_{evp}}$$

Amount of the Liquid in the system

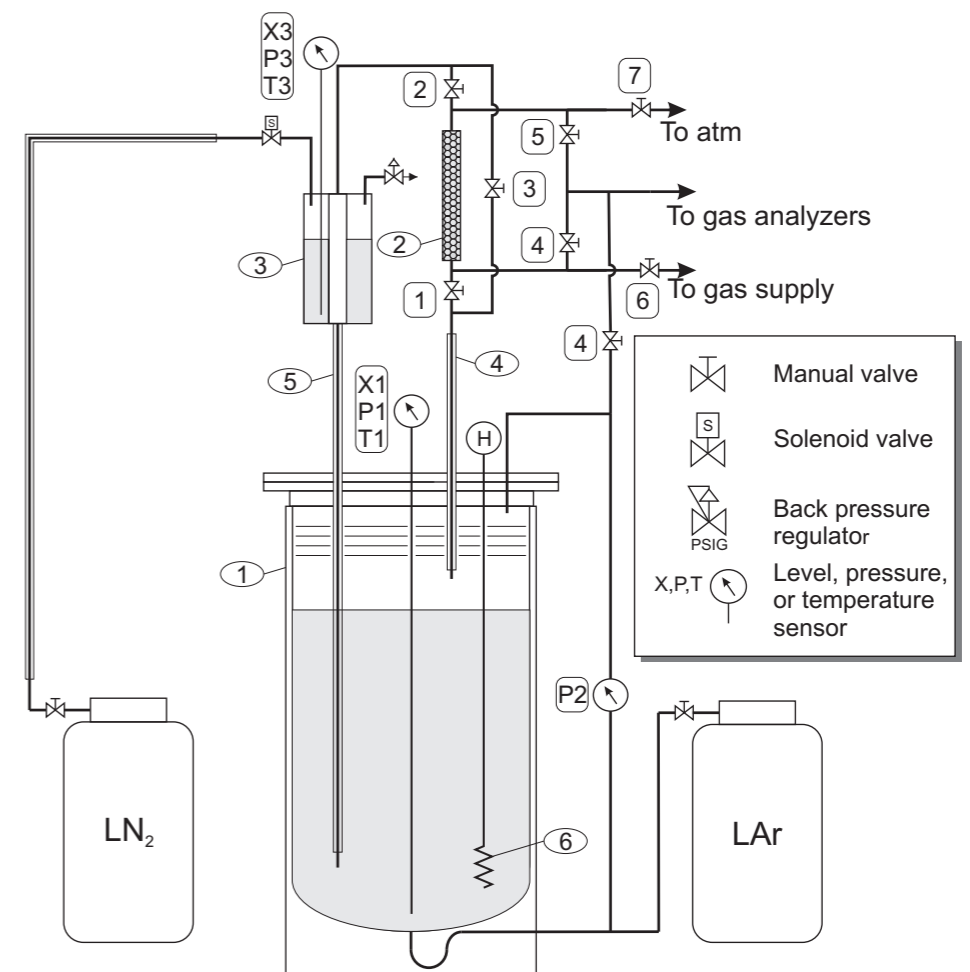
Evaporation rate of the system determined by the heat input

$$k_s = \frac{1}{\tau_{clean}}$$

Time constant of the impurity concentration

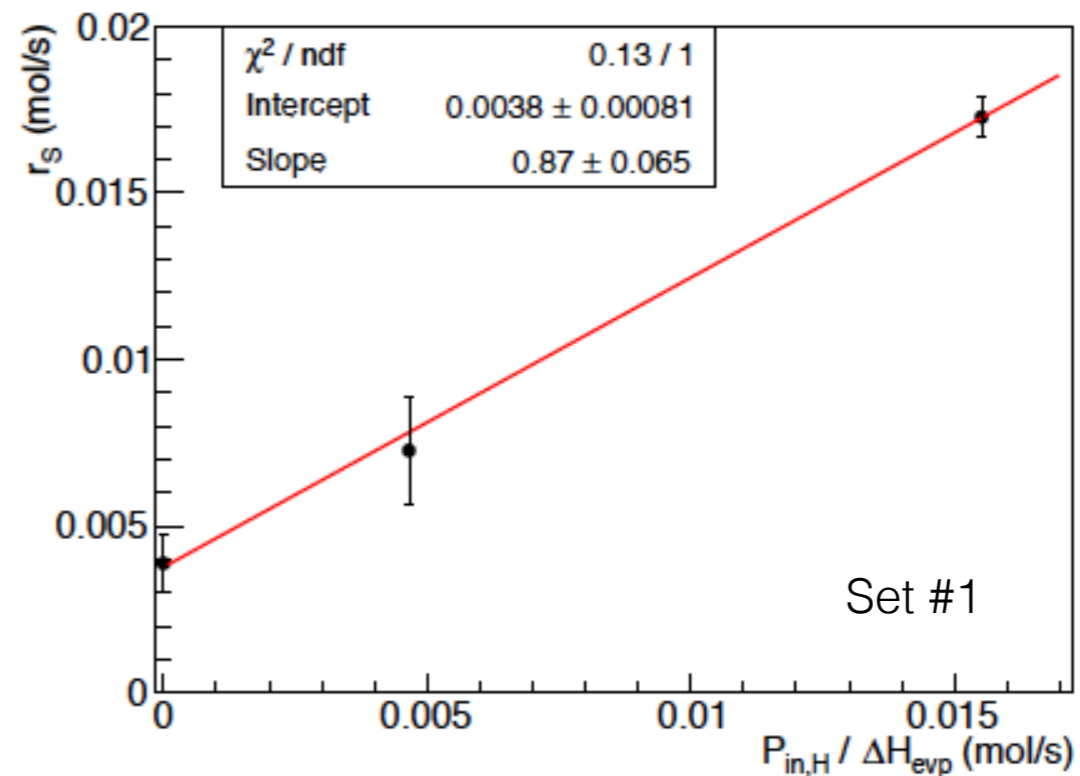
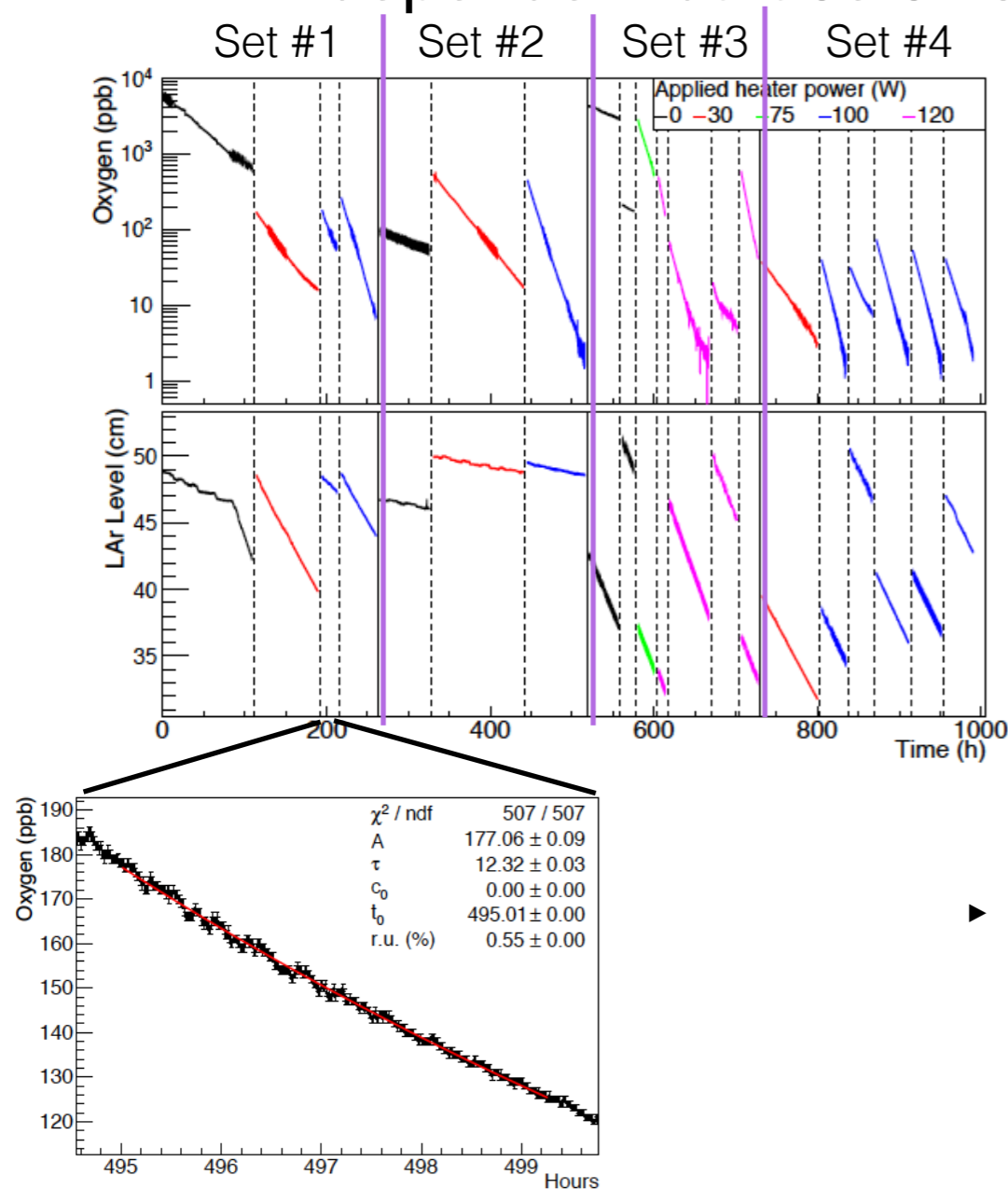
BNL 20-L LAr Test Stand

- For studying basic properties of LAr: measured longitudinal diffusion of electrons (NIMA 816 (2016) 160)
- Gas purification only
- Additional heating power can be varied 0-150 W
- Oxygen and water concentrations measured by sampling LAr into gas analyzers (0.2 ppb precision)



Henry's Coefficient for Oxygen

- Data used for analysis selected based on slow control data (LAr level, heater temperature, etc.)
- Cleaning rates measured with different heating powers
- 4 independent datasets contained in the analysis

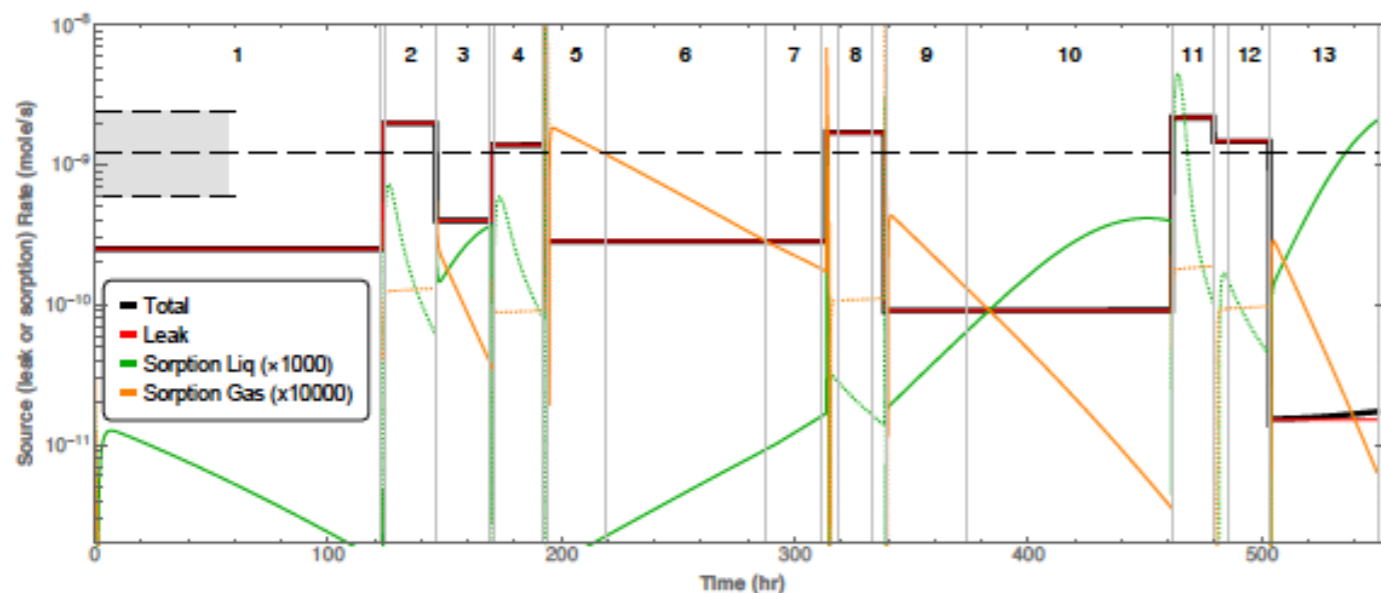
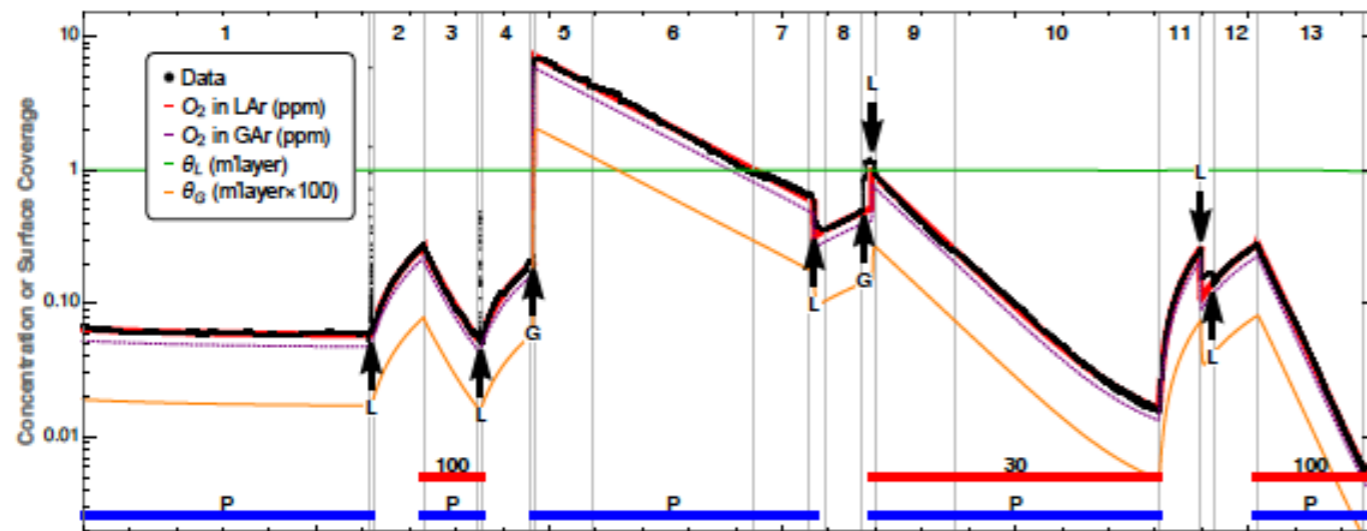


- Henry's coefficient by the model including systematics, consistent with literature

$$H_{xx} = 0.84^{+0.09}_{-0.05}$$

Additional application Numerical fit to the data

- ▶ The full model is numerically fitted to the data
- ▶ The measured Henry's coefficient is used;
- ▶ The purification off regions also fitted



- ▶ The leak rate can be determined:
 - ▶ $\sim 10^{-9}$ mol/s
- ▶ It is further reduced when heating power is increased.

Keep Impurity Away from LAr- Necked Baffle

- The dependence of leak rate on the input heating power can be explained by a simple diffusion model:

- The larger r_{evp} (higher heating power) or smaller cross section area (A_c)
- The lower concentration in the gas

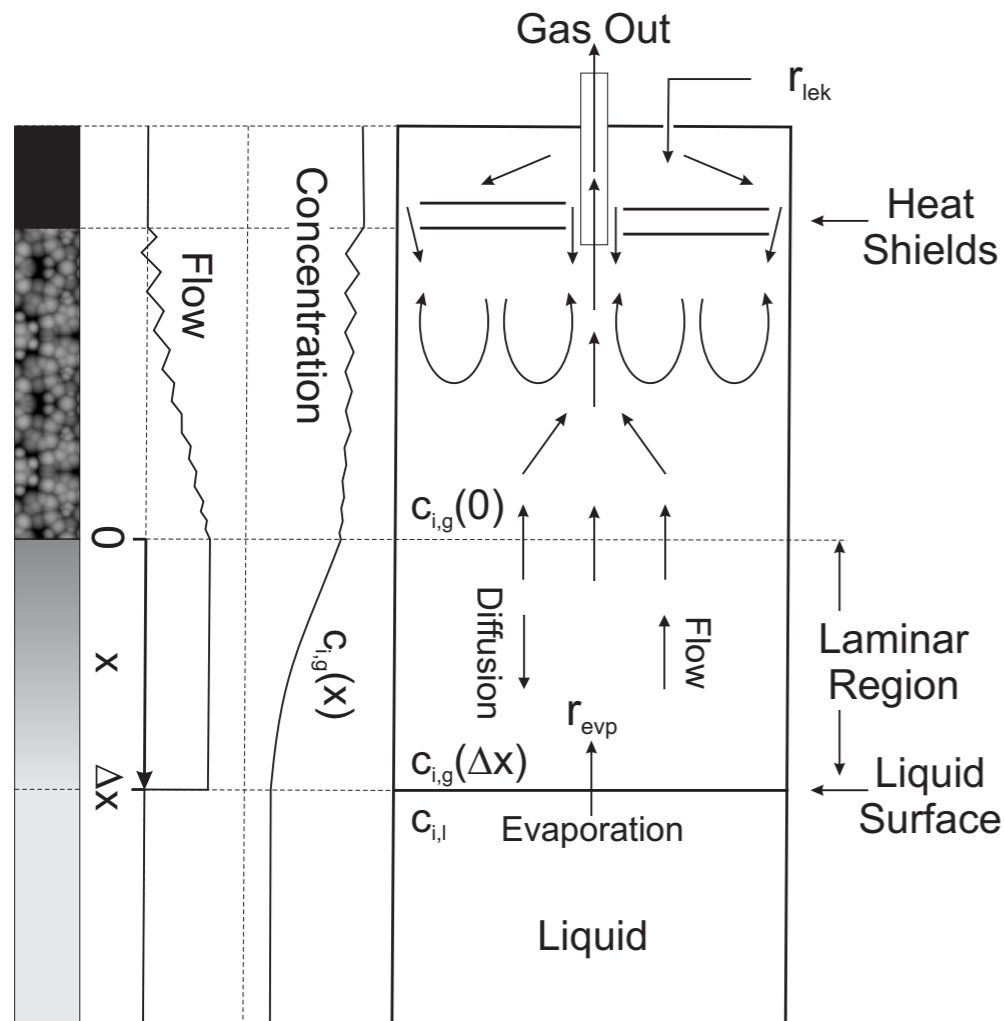
$$c_{i,g}(x) = c_{i,g}(0) \cdot e^{-\frac{r_{evp} \cdot V_m \cdot x}{D \cdot A_c}}$$

r_{evp} , evaporation rate

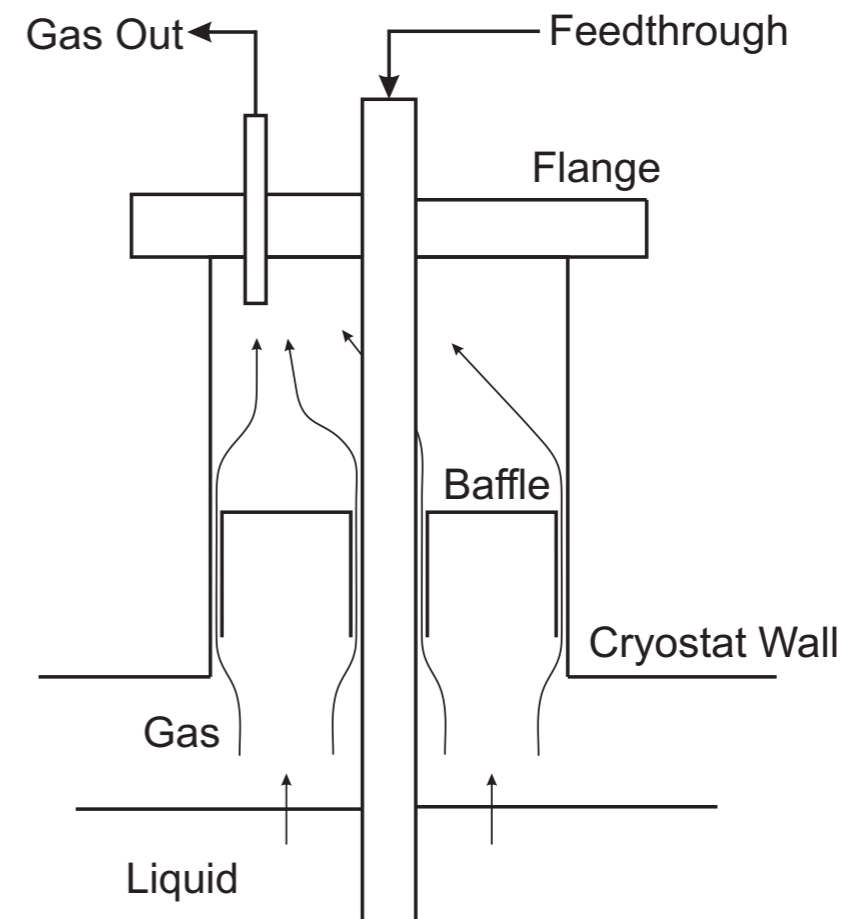
V_m , mole volume of GAr

A_c , cross sectional area perpendicular to the flow direction

D , diffusion coefficient of the impurity

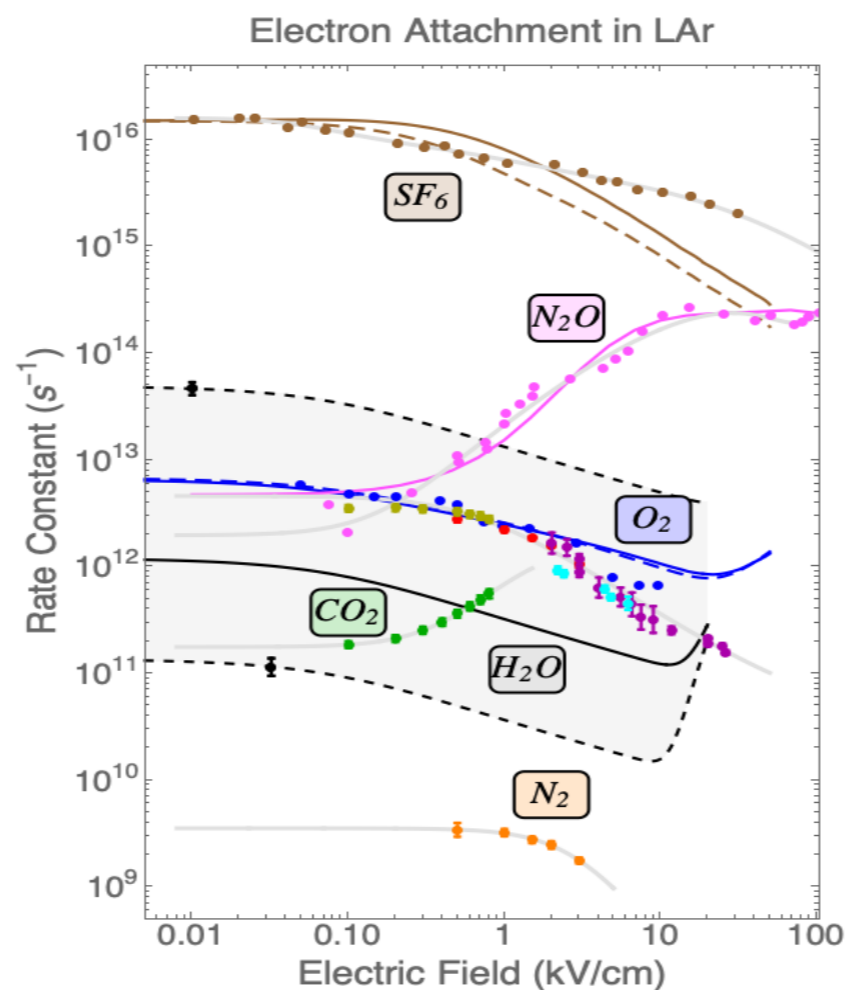


- Adding a necked baffle near the top region is expected to prevent impurities from reaching the LAr surface



Future Work on Impurities

- Understand water impurity with more data; all other impurities
- Verification of the baffle idea
- Electron attachment rate
- Electron lifetime
 - - vs. impurity concentration
 - - vs. E-field



$$n(x_i, t) = n_0 e^{-k_A x_i t} \quad \text{for mole fraction } x_i \text{ of impurity } i$$
$$n(t) = n_0 \sum_i n(x_i, t) \quad \text{for all impurities}$$

The new system-LArFCS

- Design for LArTPC field response measurement
- 260 Liter LAr Volume
 - 22" ID + 40" depth
 - Sufficient for small LArTPC
- Quick turn-round time of ~1 week with ultra-high purity (<1ppb) by gas purification
- Cryogenic operation studies last year
- Ideal place for future impurity study and other LArTPC measurements



Summary

- A mathematical model for impurities in LAr is constructed and validated with data (submitted to NIM, arXiv:2009.10906,)
- It predicts a way of measuring the Henry's coefficient for an impurity in argon.
 - The measured Henry's coefficient is consistent with literature;
- It suggests adding a necked baffle will help in reducing impurity concentrations in the detector.
- More studies are expected to come about with the new LArFCS system.

LArFCS Operation

▸ System Leak Check

- Our leak detector was not working, borrowed one
- Leak check, dominate leak at the main seal
- After tightening the bolts on the main flange, 1.7×10^{-5} Torr vacuum achieved on the top flange
- Our detector was fixed
- Expecting LAr this week

